Edge Magnetic Field in the xxz Spin-1/2 Chain

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The critical behavior associated with a transverse magnetic field applied at the edge of a semi-infinite xxz S=1/2 chain is calculated using field theory techniques. Contrary to a recent claim, we find that the long-time behavior is given by a renormalization group fixed point corresponding to an infinite field which polarizes the spin at the edge. The zero temperature entropy and position-dependent magnetization are calculated.

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There has recently been considerable interest in boundary critical behavior associated with various quantum impurity problems. In particular, it was shown by Kane and Fisher [1] that even a weak scattering potential in a repulsive Luttinger liquid effectively renormalizates to infinity at low energies so that the transmission coefficient vanishes. Independently, the essentially equivalent problem of a single impurity in an S=1/2 Heisenberg chain, which is equivalent to the spinless Luttinger liquid, was studied [2]. It was concluded that an arbitrarily small weakening of a single exchange coupling causes this coupling to renormalize to 0 giving a fixed point corresponding to a broken chain. In the bosonization approach, the infrared fixed point corresponds to a Dirichlet boundary condition, $\phi(0) =$ constant, on the boson field. It is generally believed that only in the case of a spinful Luttinger liquid, where two boson fields must be introduced, does a non-trivial fixed point occur.

A problem which is closely related to these ones involves a transverse magnetic field, h, applied at the end of a semi-infinite chain with a free boundary condition:

$$H = J\sum_{i=0}^{\infty}[S^x_iS^x_{i+1} + S^y_iS^y_{i+1} + \gamma S^z_iS^z_{i+1}] - hS^x_0. \tag{1}$$

The integrability of this model was shown in [3]. The continuum limit of this model, given below, can be written in terms of a boundary sine-Gordon field theory and describes a particle in a periodic potential coupled to a dissipative environment [4]. In the case $\gamma = 0$, the connection of the dissipation model with the spin-chain problem was exploited in [5], leading to a mapping into a free electron problem and thus an explicit solution in the continuum limit. The integrability of the boundary sine-Gordon model was shown in [6]. Further work has appeared on the continuum limit bosonized form [7,8]. The connection of this boundary sine-Gordon model with the problem of an impurity in an infinite Luttinger liquid was pointed out in [1] and [9]. The integrability of the boundary sine-Gordon model was used to obtain exact results on the impurity in the infinite Luttinger liquid in [10]. It was recently claimed [11] that both the $h = 0$ and $h = \infty$ fixed points in the spin chain model are unstable and instead, the system renormalizes to some sort of non-trivial intermediate h fixed point analogous to the behavior in the overscreened Kondo problem. If true, this would have important consequences for both the Luttinger liquid and quantum dissipation problems.

The purpose of this note is to solve for the critical properties of this spin-chain problem by an extension of the methods used in [2]. We conclude that the infinite field fixed point is stable along the entire xxz critical line $-1 < \gamma < 1$. This fixed point corresponds to a boundary condition $S^x_0 =$ constant. In bosonization language this corresponds to a Neumann boundary condition, $d\phi/dx(0) = 0$. At the isotropic point, $\gamma = 1$, the edge field is exactly marginal and a line of fixed points occurs. Our conclusion is consistent with the earlier calculations of Guinea et al. [4,5] but disagrees with the recent results of [11]. We argue that the different conclusion reached in [11] was due to a misinterpretation of the precise meaning of the infinite field fixed point. As further applications of the Neumann boundary condition, we calculate the zero temperature impurity entropy and $< S^x_j >$, showing that the latter exhibits universal oscillations which decay into the chain with a power law.

The standard bosonization technique (see for example [12]) allows us to represent the spin operators in terms of a boson field, ϕ with Lagrangian density:

$$\mathcal{L} = (1/2)[(\partial_t\phi)^2 - (\partial_x\phi)^2]. \tag{2}$$

(We set the spin-wave velocity to 1.) The long time and distance behavior of the spin operators corresponds to separate uniform and staggered components:

$$\begin{aligned} S^z_j &\approx (1/2\pi R)\partial\phi/\partial x + A(-1)^j \sin\phi/R \\ S^-_j &\approx e^{i2\pi R\tilde{\phi}}\left[B\cos\phi/R + C(-1)^j\right]. \end{aligned} \tag{3}$$

Here $\tilde{\phi}$ is the dual field, defined by splitting ϕ up into left and right moving terms:

$$\phi(t,x) = \phi_L(t+x) + \phi_R(t-x), \quad \tilde{\phi}(t,x) = \phi_L(t+x) - \phi_R(t-x). \tag{4}$$

ϕ is regarded as an angular variable on a circle of radius R given in terms of the exchange anisotropy parameter, γ, by:

$$R = \sqrt{(1/2\pi) - (1/2\pi^2)\cos^{-1}\gamma}. \tag{5}$$

Along the xxz critical line:

$$0 < R < 1/\sqrt{2\pi}. \tag{6}$$

Only the first amplitude in Eq. (3) is a universal function of R. The other constants A, B, C are non-universal. With an appropriate choice of ultraviolet regularization scheme (and the lattice spacing and spin-wave velocity set to 1),

$$< S_i^x S_j^x > \rightarrow \frac{C^2(-1)^{i-j}}{2|i-j|^{2\pi R^2}}. \tag{7}$$

Thus the (γ-dependent) constant, C, can be determined from a numerical calculation of this correlation function. An exact result for the amplitude of the correlation function was conjectured recently [13]:

$$C(\gamma) = \frac{(1+\xi)}{2}\left[\frac{\Gamma(\frac{\xi}{2})}{2\sqrt{\pi}\Gamma\left(\frac{1}{2}+\frac{\xi}{2}\right)}\right]^{\eta/2} \times \exp\left\{-(1/2)\int_0^\infty \frac{dt}{t}\left(\frac{\sinh(\eta t)}{\sinh(t)\cosh[(1-\eta)t]} - \eta e^{-2t}\right)\right\}, \tag{8}$$

where $\eta \equiv 2\pi R^2$ and $\xi \equiv \eta/(1-\eta)$. This function is plotted in Figure 1. [It goes to .5 at $\gamma \rightarrow -1$ and diverges as $(1-\gamma)^{-1/8}$ as $\gamma \rightarrow 1$.] As we shall see below, the same constant C will apear in $< S_j^x >$ in the presence of a boundary field.

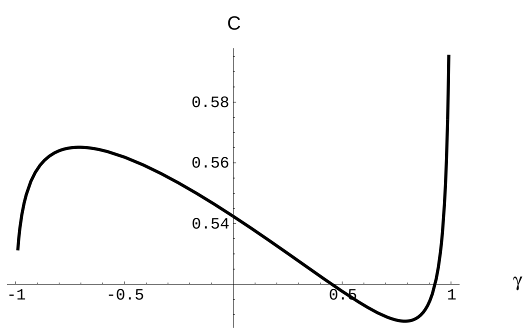

FIG. 1. The amlplitude, C appearing in the bosonization formula of Eq. (3), as a function of the anisotropy parameter, γ, defined in Eq. (1).

It was shown in [2] that free boundary conditions on the spins at $x=0$ correspond to a Dirichlet boundary condition on the boson field,

$$\phi(0) = 0. \tag{9}$$

(The value of the constant follows from requiring that $< S_j^z >= 0$.) To calculate Green's functions or RG flows at this fixed point we regard this boundary condition as relating ϕ_L and ϕ_R:

$$\phi_R(t,0) = -\phi_L(t,0). \tag{10}$$

In fact, this boundary condition allows us to regard $\phi_R(x)$ as the analytic continuation of $\phi_L(x)$ to the negative x axis:

$$\phi_R(t,x) = -\phi_L(t,-x). \tag{11}$$

This allows a straightforward evaluation of Green's functions [2].

Now we consider the effect of the edge magnetic field. The staggered component of S_0^x gives an extra boundary term in the free boson Hamiltonian:

$$H_B = -\text{constant} \cdot h \cos 2\pi R\tilde{\phi}(0). \tag{12}$$

Using the fact that we have a free boundary condition, we may equivalently write this as:

$$H_B = -\text{constant} \cdot h \cos[4\pi R\phi_L(0)]. \tag{13}$$

This has a scaling dimension:

$$d = 2\pi R^2. \tag{14}$$

Since $d < 1$ along the entire xxz critical line this is a relevant boundary interaction. At the antiferromagnetic Heisenberg point $\gamma = 1$, it is marginal. We return to this special case below. The simplest possibility to assume is that h renormalizes to ∞ in the infrared. From Eq. (12) this implies a Neumann boundary condition

$$\tilde{\phi}(0) = \phi_L(0) - \phi_R(0) = 0, \tag{15}$$

and hence $\partial\phi/\partial x = \partial\tilde{\phi}/\partial t = 0$. What this assumption means in practical terms is that Green's functions involving spatial locations far from the chain-end compared to a crossover length scale ξ (given below) and long time intervals compared to $1/\xi$ will be given by the free boson model with the Neumann boundary condition. To check the consistency of this assumption, we should calculate the scaling dimension of all operators allowed by symmetry which could be added to the effective Hamiltonian. Our assumption is consistent if these are all irrelevant, $d > 1$. Imposing the boundary condition, we may write the spin operator at the origin as:

$$S_0^x \approx C + B \cdot \cos(2\phi_L/R) \tag{16}$$

The operator $\cos(2\phi_L/R)$ is certainly allowed by symmetry in the effective Hamiltonian, since it occurs in S_0^x. It has scaling dimension:

$$d = 1/2\pi R^2 > 1, \tag{17}$$

and is therefore irrelevant. This is a natural result given the interpretation of the Neumann boundary condition as corresponding to infinite field. Applying an additional field at any sites near the chain edge shouldn't destabilize the fixed point.

The marginal operator $\partial\tilde{\phi}/\partial x$ is forbidden by the symmetry of rotation by π around the x-axis, which is still a good symmetry in the presence of the magnetic field. This takes $\tilde{\phi} \to -\tilde{\phi}$. Thus only irrelevant operators, $(\partial\tilde{\phi}/\partial x)^2$, $\cos 2n\phi_L/R$ (for $n = 1, 2, 3, \ldots$) are allowed. Hence the infinite field fixed point is stable. It is thus very natural to assume that even a very small field will renormalize to ∞ so that the Neumann boundary condition describes the long-time behavior. Indeed it is difficult to imagine what a non-trivial fixed point (neither Dirichlet nor Neumann) would look like. In fact, it can be proven that Dirichlet and Neumann boundary conditions are the only conformally invariant ones in a theory containing a single periodic boson, for generic R [14]. Hence, there can be no other fixed points if we assume that they correspond to conformally invariant boundary conditions.

Note that if we had ignored the Neumann boundary condition and considered the bulk operator $\cos(\phi/R)$ we would have obtained the dimension $1/4\pi R^2$, which is precisely $1/2$ the correct value. This obeys $d < 1$ along the xxz critical line for $\gamma > 0$ which would imply that the operator was relevant and the infinite field fixed point was unstable. The infinite field limit *does not* give a problem equivalent to the initial one because the boundary conditions have changed from Dirichlet to Neumann. The result is that a magnetic field (in the x-direction) becomes irrelevant with Neumann boundary conditions while it was relevant with Dirichlet boundary conditions. It is instructive to contrast the RG behavior of the present problem with a spin chain version of the 2-channel Kondo problem of the type treated in [2] where we consider the Heisenberg model ($\gamma = 1$) on the infinite line with a coupling, J_K between sites 0 and ± 1 which is different than the bulk coupling, J. In that case the $J_K = \infty$ fixed point really is equivalent to the $J_K = 0$ fixed point because the three strongly coupled spins form an effective $S = 1/2$ spin at $J_K = \infty$ and the neighboring spins on sites ± 2 obey free boundary conditions with no coupling to the effective spin in that limit. This follows because the exchange coupling between sites 1 and 2 (and also between sites -1 and -2) maps the low energy states of

the strongly coupled 3-spin complex into high energy states, so, using second order degenerate perturbation theory, the effective coupling to sites ± 2 is of order $J^2/J_K \to 0$. By contrast, in the magnetic field case the $h = \infty$ limit effectively eliminates the spin $\vec{S}_0$ but the effective field acting on $\vec{S}_1$ does not go to 0, but rather to a finite value, $-J/2$. Thus this situation is not equivalent to $h \to 0$, contrary to the statement in [11]. Instead, we must regard the infinite field limit as a different fixed point corresponding to a Neumann boundary condition in the field theory.

The "groundstate degeneracy" (exponential of the zero temperature entropy) for Dirichlet and Neumann fixed points is [15]

$$g_D = 1/\sqrt{2\sqrt{\pi}R}, \quad g_N = \sqrt{\sqrt{\pi}R}. \tag{18}$$

We see that $g_N < g_D$ for all $R < 1/\sqrt{2\pi}$, that is along the entire xxz critical line. Thus our assumption of renormalization from Dirichlet to Neumann fixed points is consistent with the g-theorem [16].

Next, as another application of the Neumann boundary condition, we calculate the long- distance behavior of $< S_j^x >$. Other Green's functions can be calculated the same way. We use our bulk bosonization formulas, Eq. (3) and use the Neumann boundary condition to regard ϕ_R as the analytic continuation of ϕ_L:

$$\phi_R(x) = \phi_L(-x). \tag{19}$$

Hence:

$$S_j^x \approx \cos 2\pi R[\phi_L(x) - \phi_L(-x)] \cdot \left\{B \cos\{[\phi_L(x) + \phi_L(-x)]/R\} + C(-1)^j\right\} \tag{20}$$

Thus

$$< S_j^x > \to C(-1)^j < e^{i2\pi R\phi_L(x)} e^{-i2\pi R\phi_L(-x)} > = \frac{C(-1)^j}{(2j)^{\pi R^2}}. \tag{21}$$

This formula is only valid outside a cross over length which can be estimated from the renormalization group, in the case of a weak field as:

$$\xi \propto (J/h)^{1-2\pi R^2}. \tag{22}$$

The amplitude, C is determined in the bulk theory [for example from the behavior of the correlation function in the infinite system, Eq. (7)] and is independent of the strength of the edge field, h. This reflects the fact that the system flows to a universal fixed point regardless of the size of h.

Finally, we consider the isotropic Heisenberg antiferromaget, $\gamma = 1$, $R = 1/\sqrt{2\pi}$. In this case the direction of the applied field is immaterial so we choose the z-direction. This case turns out to be very similar to the case of arbitrary γ between -1 and +1 with the field in the z-direction so we consider that more general situation. The magnetic field gives the term in the bosonized Hamiltonian (using the Dirichlet boundary condition):

$$H_B = -h\alpha \cdot \partial\phi_L/\partial x(0), \tag{23}$$

where α is a non-universal constant of O(1). Actually, this form of the prefactor is only valid at small h. For larger h it must be replaced by some non-universal function of h. Adding this to the free boson Hamiltonian leaves a free boson theory which can be solved exactly. This perturbation is exactly marginal, leading to a line of fixed points. Using the Dirichlet boundary condition to eliminate the right-movers, the full Hamiltonian can be written:

$$H = \int_{-\infty}^{\infty} (d\phi_L/dx)^2 - h\alpha d\phi_L/dx(0). \tag{24}$$

This boundary term can be adsorbed into a discontinuity of the field ϕ_L at the origin:

$$\phi_L' \equiv \phi_L - h\alpha\theta(x)/2, \tag{25}$$

where θ is the step function. Applying this shift to the Dirichlet boundary condition we can write:

$$< S_j^z > \to B(-1)^j < \sin(\phi_L'(x) - \phi_L'(-x) + h\alpha/2)/R > . \tag{26}$$

For small h this gives:

$$< S^z_J >\propto \frac{h(-1)^j}{|j|^{1/4\pi R^2}}. \tag{27}$$

The exponent equals 1/2 at the isotropic point, $2\pi R^2 = 1$, in agreement with the previous calculation, Eq. (21). Note that in this case the prefactor varies with h, corresponding to a line of fixed points. The boundary states at the isotropic point have been discussed in [7]. In particular, it was shown that the line of fixed points terminates at the Neumann fixed point, corresponding to infinite field.

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